# AIR RESOURCES LABORATORY

# SEMINAR

## Demonstration of an Operational Multiscale Numerical Air Quality Prediction System

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Abstract

An operational multiscale numerical air quality prediction system has been developed and deployed by a team of atmospheric scientists at MCNC-North Carolina Supercomputing Center in Research Triangle Park, NC. Building on prototype work conducted in 1998 and 1999, the team is successfully delivering timely and useful tropospheric ozone forecasts in support of the ongoing Texas AQS-2000 Field program. These forecasts are being used daily by the forecasters, aircraft operations groups, and experimental atmospheric chemists involved in the field program, to assist understanding both the large-scale and high-resolution potential for ozone formation up to 48 hours in advance. Additionally, forecasts provide numerical ozone guidance to the ozone forecast groups at the Texas Natural Resources Conservation Commission (TNRCC) and the North Carolina Department of Environment and Natural Resources (NC-DENR).

The forecast system consists of three models coupled one-way in real-time, each running on multiple scales and communicating via the MCNC-EPA Models-3 I/O API, which transparently provides user selected combinations of Parallel-Virtual Machine (PVM) mailbox based data exchange/coordination and netCDF disk-based files. The system is run twice daily, at 00z and 12z, at resolutions of 45km, 15km and 5km.

The PSU/NCAR MM5V2.12 is the meteorological forecast part of the modeling system. For this project, it is principally driven with NCEP Eta-analyses for large-scale initial conditions, and Eta forecasts for large-scale boundary conditions. MM5 has been augmented by MCNC's MCPL output module, which provides flexible and configurable I/O API output in a form ready for coupling to the emissions and chemical-transport models.

MCNC's Sparse-Matrix Operator Kernel Emissions (SMOKE) modeling system is used to provide emissions forecasts. SMOKE is a high-performance emissions modeling system built around sparse matrix algorithms and the I/O API. It is driven by emissions inventories for biogenic, point, area, and mobile sources, which are then modulated by the real-time MM5 forecast meteorology at all relevant scales.

The Multiscale Air Quality Simulation Platform (MAQSIP) is a modular science-process, generalized vertical coordinate-based atmospheric chemistry and transport model. MAQSIP is closely related to EPA's Models-3, the first version having been designed and built by MCNC Environmental Programs scientists in the mid-1990's for EPA to use as a Models-3 prototype. MAQSIP's current real-time configuration includes an advanced version of the 35-species Carbon-Bond IV gas-phase chemical mechanism, a cloud-chemistry package consisting of a chemical version of the Kain-Fritsch deep convective parameterization, a mass flux based shallow convective scheme, a resolved cloud chemistry scheme, and a sub-grid-scale cloud chemistry scheme. Clouds act to transport, transform, and, if precipitating, remove species from the atmosphere, as well as to modify the solar actinic flux critical for photochemical ozone formation. Vertical turbulent diffusion and 3-D advection, dry and wet deposition, along with all other major relevant physical and chemical processes, are treated in the model. MAQSIP has undergone significant improvements and code optimization/parallelization since first being developed.

The seminar will consist of an operational demonstration of the system as it is currently running in real-time, a "tour" of forecast products generated by MCNC's Package for Analysis and Visualization of Environmental Data (PAVE) and VIS5D, conceptual data-flow diagrams, an overview of the lower level software layers constructed to manage the system (including MCNC's I/O API), handouts with relevant background conference and journal articles, and a question and answer session.